

From Quantum Dynamics to the Canonical Distribution – General Picture and a Rigorous Example¹

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Abstract

Derivation of the canonical (or Boltzmann) distribution based only on quantum dynamics is discussed. Consider a closed system which consists of mutually interacting subsystem and heat bath, and assume that the whole system is initially in a pure state (which can be far from equilibrium) with small energy fluctuation. Under the “hypothesis of equal weights for eigenstates”, we derive the canonical distribution in the sense that, at sufficiently large and typical time, the (instantaneous) quantum mechanical expectation value of an arbitrary operator of the subsystem is almost equal to the desired canonical expectation value. We present a class of examples in which the above derivation can be rigorously established without any unproven hypotheses.

It is often said that the principles of equilibrium statistical physics have not yet been justified. It is not clear, however, what statement should be regarded as the ultimate justification. Recalling the astonishingly universal applicability of equilibrium statistical physics, it seems likely that there are many independent routes for justification which can be equally convincing and important [1, 2]. In the present paper, we concentrate on one of the specific scenarios for obtaining canonical distributions from quantum dynamics [3].

Outline of the work: Let us outline our problem and the main result. We consider an isolated quantum mechanical system which consists of a subsystem and a heat bath. The subsystem is described by a Hamiltonian H_S which have arbitrary nondegenerate eigenvalues $\varepsilon_1, \dots, \varepsilon_n$. For convenience we let $\varepsilon_{j+1} > \varepsilon_j$ and $\varepsilon_1 = 0$. The heat bath is described by a Hamiltonian H_B with the density of states $\rho(B)$. The inverse temperature of the heat bath at energy B is given by the standard formula $\beta(B) = d \log \rho(B) / dB$. We assume (as usual) $\beta(B)$ is positive and decreasing in B . The density of states $\rho(B)$ is arbitrary except for a fine structure that we will impose on the spectrum of H_B .

The coupling between the subsystem and the heat bath is given by a special Hamiltonian H' which almost conserves the unperturbed energy and whose magnitude is $\|H'\| \sim \lambda$. We assume $\Delta\varepsilon \gg \lambda \gg \Delta B$, where $\Delta\varepsilon$ is the minimum spacing of the energy levels of H_S , and ΔB is the maximum spacing of that of H_B . These conditions guarantee a weak coupling between the subsystem and the bath, as well as macroscopic nature of the bath. The Hamiltonian of the whole system is $H = H_S \otimes \mathbf{1}_B + \mathbf{1}_S \otimes H_B + H'$, where $\mathbf{1}_S$ and $\mathbf{1}_B$ are the identity operators for the subsystem and the heat bath, respectively.

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Suppose that the whole system is initially in a pure state $\Phi(0)$ which has an energy distribution peaked around (but not strictly concentrated at) E . It is possible to treat mixed states as well, but such extensions are not essential. For an operator A of the subsystem, we denote its quantum mechanical expectation value at time t as

$$\langle A \rangle_t = \langle \Phi(t), (A \otimes \mathbf{1}_B) \Phi(t) \rangle, \quad (1)$$

where $\langle \cdot, \cdot \rangle$ stands for the inner product, and $\Phi(t) = e^{-iHt} \Phi(0)$ is the state at time t . Note that $\langle \cdot \cdot \rangle_t$ is a mixed state on the subsystem. Our main result is the derivation of the canonical distribution in the sense that

$$\langle A \rangle_t \simeq \langle A \rangle_{\beta(E)}^{\text{can}} \quad \text{for any } A, \quad (2)$$

holds [4] for sufficiently large and typical t , where $\langle A \rangle_{\beta}^{\text{can}} = \text{Tr}_S[Ae^{-\beta H_S}] / \text{Tr}_S[e^{-\beta H_S}]$ is the canonical expectation value. We show that (2) holds for rather general systems under the “hypothesis of equal weights for eigenstates.” For a special class of models, we prove (2) rigorously without any unproven hypotheses.

We note the following points about the present derivation of the canonical distribution. (i) We do not introduce any probability distributions by hand. (ii) We do not make use of the microcanonical distribution. (iii) We do not perform any time averaging. (iv) We do not take any limits such as making the bath infinitely large or the coupling infinitesimally small. (v) Quantum mechanics seems to play essential roles.

In the present paper, we describe our main results and basic idea of proofs, leaving details to [5]. We also briefly discuss possible extension of the present scenario to more general systems.

Coupling: We diagonalize the (partial) Hamiltonians as $H_S \Psi_j = \varepsilon_j \Psi_j$ with $j = 1, \dots, n$, and $H_B \Gamma_k = B_k \Gamma_k$ with $k = 1, \dots, N$, where Ψ_j, Γ_k are normalized. We will impose a fine structure on the spectrum $\{B_k\}$ when we discuss our rigorous results.

When the coupling H' is absent, the total Hamiltonian $H_0 = H_S \otimes \mathbf{1}_B + \mathbf{1}_S \otimes H_B$ has eigenstates $\Theta_{(j,k)} = \Psi_j \otimes \Gamma_k$ with eigenvalues $U_{(j,k)} = \varepsilon_j + B_k$. We now introduce a new index $\ell = 1, \dots, nN$ for Θ and U . The index ℓ is in a one-to-one correspondence with the original index (j, k) such that $U_{\ell+1} \geq U_{\ell}$ holds for $\ell = 1, \dots, nN - 1$. We define the coupling Hamiltonian H' as

$$\langle \Theta_{\ell}, H' \Theta_{\ell'} \rangle = \begin{cases} \lambda/2, & \text{if } |\ell - \ell'| = 1; \\ 0, & \text{otherwise,} \end{cases} \quad (3)$$

with a constant $\lambda > 0$. The Hamiltonian H' describes scattering processes which almost conserve the unperturbed energy.

Eigenstates—main idea: Let Φ_E be a normalized eigenstate of the total Hamiltonian $H = H_0 + H'$ with energy E . Expanding it as $\Phi_E = \sum_{\ell=0}^{nN} \varphi_{\ell} \Theta_{\ell}$, the Schrödinger equation $E\Phi_E = H\Phi_E$ is written as

$$E\varphi_{\ell} = \frac{\lambda}{2}(\varphi_{\ell-1} + \varphi_{\ell+1}) + U_{\ell}\varphi_{\ell}, \quad (4)$$

with $\varphi_0 = \varphi_{nN+1} = 0$. This may be regarded as the Schrödinger equation for a single quantum mechanical “particle” on a “chain” $\{1, 2, \dots, nN\}$ under the monotone “potential” U_ℓ .

The eigenstates of (4) with a constant $U_\ell = U$ are $\varphi_\ell = e^{\pm i k \ell}$ with $k = \cos^{-1}[(E - U)/\lambda]$ if $|E - U| < \lambda$, and $\varphi_\ell = e^{\pm \kappa \ell}$ (or $\varphi_\ell = (-1)^\ell e^{\pm \kappa \ell}$) with $\kappa = \cosh^{-1}[|E - U|/\lambda]$ if $E - U > \lambda$ (or $E - U < -\lambda$). Since our “potential” U_ℓ varies slowly in ℓ , the quasi-classical argument [6] suggests that generally φ_ℓ takes appreciable values in the “classically accessible region” (which consists of ℓ such that $|E - U_\ell| \lesssim \lambda$), and is negligible outside the region. More precisely we expect that, for general E , we can write $|\varphi_\ell|^2 \approx f(E - U_\ell)$ with a (E dependent) function $f(\tilde{E})$ which is nonnegligible only for $|\tilde{E}| \lesssim \lambda$. In terms of the original index, this reads

$$|\varphi_{(j,k)}|^2 \approx f[E - (\varepsilon_j + B_k)]. \quad (5)$$

To see consequences of (5), we take an arbitrary operator A of the subsystem, and denote its matrix elements as $(A)_{j,j'} = \langle \Psi_j, A \Psi_{j'} \rangle$. By using (5) and noting that $\Delta\varepsilon \gg \lambda \gg \Delta B$, we find

$$\begin{aligned} \langle \Phi_E, (A \otimes \mathbf{1}_B) \Phi_E \rangle &= \sum_{j,j'=1}^n \sum_{k=1}^N \varphi_{(j,k)}^* \varphi_{(j',k)} (A)_{j,j'} \\ &\simeq \frac{\sum_{j,k} |\varphi_{(j,k)}|^2 (A)_{j,j}}{\sum_{j,k} |\varphi_{(j,k)}|^2} \\ &\simeq \frac{\sum_j \int dB \rho(B) f(E - \varepsilon_j - B) (A)_{j,j}}{\sum_j \int dB \rho(B) f(E - \varepsilon_j - B)} \\ &\simeq \frac{\sum_j \rho(E - \varepsilon_j) (A)_{j,j}}{\sum_j \rho(E - \varepsilon_j)} \\ &\simeq \langle A \rangle_{\beta(E)}^{\text{can}}, \end{aligned} \quad (6)$$

where the final estimate follows by Taylor expanding $\rho(E - \varepsilon_j)$ as usual.

The relation (6) states that the expectation value in an eigenstate is equal to the desired canonical expectation value. This is the key estimate in the present work, and the rest of our results follow from relatively general (and standard) arguments. Although we have restricted our discussion to the H' of the form (3), we expect (and can partially prove [5]) that the property (5) holds for general eigenstates of systems with more general couplings H' . This may be called [5] the “hypothesis of equal weights for eigenstates”, from which we may get the key estimate (6) and its consequences.

Eigenstates—rigorous result: We will precisely state the assumption on H_B , and describe a rigorous estimate corresponding to (6). We fix an energy unit $\delta > 0$ (which may be much smaller than λ), a positive integer R , and positive integers M_1, M_2, \dots, M_R . We then introduce an integer $L \geq L_0$ (where L_0 is a constant), which will be made sufficiently large (but finite) to realize the situation where the bath is “large.” We require for each $r = 1, \dots, R$

that LM_r eigenvalues of H_B are distributed in the interval $((r-1)\delta, r\delta)$ with an equal spacing $b_r = (LM_r)^{-1}\delta$. Thus the density of states of the bath is written as $\rho(r\delta) = LM_r/\delta$.

With this special H_B , we can partially control the solution of (4) and the sums in (6) to get the following [7].

Lemma — Consider a system where H_B has the above fine structure, and the coupling H' is given by (3). We assume $\varepsilon_{j+1} - \varepsilon_j \geq 4\lambda$ for any j . Let E be an eigenvalue of the whole Hamiltonian H such that $\varepsilon_n + 2\lambda \leq E \leq B_{\max} - 2\lambda$, and Φ_E be the corresponding eigenstates. Then for any operator A of the subsystem, we have

$$\left| \langle \Phi_E, (A \otimes \mathbf{1}_B) \Phi_E \rangle - \langle A \rangle_{\beta}^{\text{can}} \right| \leq \sigma \|A\|. \quad (7)$$

Here $\sigma = 3\beta\lambda + \gamma(\varepsilon_n)^2 + cL^{-1/12}$ with $\beta = \beta(E) = d \log \rho(E)/dE$, $\gamma = |d\beta(E - \lambda)/dE|$, $\|A\| = \max_{j,j'} |(A)_{j,j'}|$, and c is a constant independent of L , E , and A .

Note that we have $\sigma \ll 1$ if (i) the coupling is weak (to have $\beta\lambda \ll 1$), (ii) $\beta(E)$ varies slowly (to have $\gamma(\varepsilon_n)^2 \ll 1$), and (iii) the level spacing of the bath is small (to have $cL^{-1/12} \ll 1$). Recall that these are the standard assumptions regarded necessary to get the canonical distribution. We have established the key estimate (6) rigorously under reasonable conditions.

Long-time average: Let $\Phi(0)$ be the initial state (of the whole system), and expand it as

$$\Phi(0) = \sum_E \gamma_E \Phi_E, \quad (8)$$

where the sum runs over the eigenvalues of H . The state at time t is given by $\Phi(t) = \sum_E e^{-iEt} \gamma_E \Phi_E$. Then the quantum mechanical expectation value (1) can be written as

$$\langle A \rangle_t = \sum_{E, E'} e^{i(E-E')t} (\gamma_E)^* \gamma_{E'} \langle \Phi_E, (A \otimes \mathbf{1}_B) \Phi_{E'} \rangle. \quad (9)$$

Since energy eigenvalues of (4) are nondegenerate, we find that the long-time average of $\langle A \rangle_t$ becomes

$$\begin{aligned} \overline{\langle A \rangle_t} &= \sum_{E'} |\gamma_{E'}|^2 \langle \Phi_{E'}, (A \otimes \mathbf{1}_B) \Phi_{E'} \rangle \\ &\simeq \sum_{E'} |\gamma_{E'}|^2 \langle A \rangle_{\beta(E')}^{\text{can}}, \end{aligned} \quad (10)$$

where $\overline{F(t)} = \lim_{T \rightarrow \infty} T^{-1} \int_0^T dt F(t)$, and we used (6) or (7) to get the final line.

Further suppose that the initial state $\Phi(0)$ has a small energy fluctuation in the sense that the coefficients $\gamma_{E'}$ is nonnegligible only for E' close to some fixed energy E . Then (10) reduces to

$$\overline{\langle A \rangle_t} \simeq \langle A \rangle_{\beta(E)}^{\text{can}}, \quad (11)$$

which states that the long-time average of the quantum mechanical expectation value is almost equal to the desired canonical expectation value [8].

An interesting example of an initial state with small energy fluctuation is

$$\Phi(0) = \Psi_n \otimes \sum_k \alpha_k \Gamma_k, \quad (12)$$

with α_k nonnegligible for k in a finite range. Note that the state (12), restricted onto the subsystem, is very far from equilibrium since n is the index for the highest energy state of the subsystem.

Approach to equilibrium: We have seen that, for the initial state with small energy fluctuation, the time-independent part in the right-hand side of (9) gives the desired canonical expectation value. The time-dependent part of (9) is a linear combination of many terms oscillating in t with different frequencies. It might happen that at sufficiently large and typical (fixed) t , these oscillating terms cancel out with each other, and $\langle A \rangle_t$ becomes almost identical to its time-independent part $\overline{\langle A \rangle}_t$.

This naive guess is strengthened by the following simple estimate of the variance.

$$\begin{aligned} \overline{(\langle A \rangle_t - \overline{\langle A \rangle}_t)^2} &= \overline{(\langle A \rangle_t)^2} - (\overline{\langle A \rangle}_t)^2 \\ &= \sum_{E_1, E_2, E_3, E_4} (\gamma_{E_1})^* \gamma_{E_2} (\gamma_{E_3})^* \gamma_{E_4} \overline{e^{i(E_1 - E_2 + E_3 - E_4)t}} \langle E_1 | A | E_2 \rangle \langle E_3 | A | E_4 \rangle \\ &\quad - \left(\sum_E |\gamma_E|^2 \langle E | A | E \rangle \right)^2 \\ &\leq \sum_{E, E'} |\gamma_E|^2 |\gamma_{E'}|^2 \langle E | A | E' \rangle \langle E' | A | E \rangle \\ &\leq n^2 \|A\|^2 \max_E |\gamma_E|^2, \end{aligned} \quad (13)$$

where we used the Dirac notation $\langle E | A | E' \rangle = \langle \Phi_E, (A \otimes \mathbf{1}_B) \Phi_{E'} \rangle$, and used the bound $\langle E | A^2 | E \rangle \leq n^2 \|A\|^2$. We also assumed the non-resonance condition for the relevant energy eigenvalues, i.e., whenever $E_1 - E_2 = E_4 - E_3 \neq 0$ holds for E_i such that $\gamma_{E_i} \neq 0$, we have $E_1 = E_4$ and $E_2 = E_3$. Although we are not able to verify the non-resonance condition for a particular given model, it is easily proved that the condition is satisfied for generic models [9]. When a large number of states equally contribute to the expansion (8), $|\gamma_E|^2$ and hence the right-hand side of (13) is very small. This means that $\langle A \rangle_t$ usually takes values very close to its average $\overline{\langle A \rangle}_t$.

Following the idea of the Chebyshev's inequality [10], this observation can be made into a rigorous statement. Instead of writing down the general theorem [5] we present its consequence for the special (but interesting) situations with the initial states (12).

Theorem — Suppose that the conditions of the Lemma hold, and the non-resonance condition is valid for energy eigenvalues with $\varepsilon_n + 2\lambda \leq E_i \leq B_{\max} - 2\lambda$. Fix an arbitrary energy E with $\varepsilon_n + 3\lambda \leq E \leq B_{\max} - 3\lambda$. Take an initial state $\Phi(0)$ of the form (12), and assume that α_k is nonvanishing only for k such that $|E - (B_k + \varepsilon_n)| \leq \varepsilon_n/2$, and satisfies $(\alpha_k)^2 \leq c'(\varepsilon_n \rho(E))^{-1}$ with an arbitrary constant $c' \geq 1$ [11]. We let $\sigma' = 3\beta\lambda + 3\gamma(\varepsilon_n)^2 +$

$cL^{-1/12} + n^2(\lambda/\varepsilon_n)^{1/3}$, where β, γ are the same as in the Lemma. Then there exists a finite $T > 0$ and a subset (i.e., a collection of intervals) $\mathcal{G} \subset [0, T]$ with the following properties. a) For any $t \in \mathcal{G}$, we have

$$|\langle A \rangle_t - \langle A \rangle_\beta^{\text{can}}| \leq \sigma' \|A\|, \quad (14)$$

for any operator A of the subsystem. b) If we denote by $\mu(\mathcal{G})$ the total length of the intervals in \mathcal{G} , we have

$$1 \geq \frac{\mu(\mathcal{G})}{T} \geq 1 - 3c' \left(\frac{\lambda}{\varepsilon_n} \right)^{1/3}. \quad (15)$$

In simpler words, \mathcal{G} is the collection of “good” time intervals, in which the quantum mechanical expectation value of *any* operator is equal to the canonical expectation value within the relative error σ' . The new factor λ/ε_n is small if the coupling is weak. Therefore under the physical conditions (i)-(iii) stated below the Lemma, both σ' and $3c'(\lambda/\varepsilon_n)^{1/3}$ in (15) are small. Then (15) says that the “good” intervals essentially cover the whole interval $[0, T]$. We thus have obtained the desired (2) for most t within the time interval $0 \leq t \leq T$. Recall that the subsystem is far from equilibrium at $t = 0$. *By using only quantum dynamics and the assumptions about the initial state, we have established an approach to the desired canonical distribution from a highly nonequilibrium state.* Although our theorem is proved only for systems with particular fine structure and special H' , the essential physics is contained in the “hypothesis of equal weights for eigenstates” and the non-resonance condition (or related weaker conditions). We expect the same scenario to work for much more general systems.

Our result is not strong enough to clarify how $\langle A \rangle_t$ approaches (or deviates from) its equilibrium value. Note that we can never expect a perfect decay to equilibrium since $\langle A \rangle_t$ is quasiperiodic in t . In a long run, $\langle A \rangle_t$ deviates from the equilibrium value infinitely often. Our theorem does guarantee that such deviations are indeed very rare for a weak (but finite) coupling. Unfortunately we do not have any meaningful estimate for T .

Irreversibility: One might question if our theorem implies the existence of an “irreversible” time evolution towards equilibrium. We believe the answer is affirmative, but we have to be careful about this delicate issue. We first stress that, exactly as in classical cases [1], whether we see irreversibility or not depends on the choice of physical quantities that we observe. We should clearly see irreversibility when (there is irreversibility and) we observe quantities which have small fluctuation in the equilibrium (and preferably in the initial state too) [12].

To get an illustrative example, we suppose n is large, and set A to be the projection onto the state Ψ_n . A has eigenvalues 0 and 1. In the initial state $\Phi(0)$ of the form (12), an observation of A does not disturb the state and one gets a definite result 1. We then wait for a sufficiently long time (required by the theorem), and once again observe A at time t . If this t does not belong to the exceptional “bad” intervals, the theorem guarantees that $\langle A \rangle_t \simeq \langle A \rangle_\beta^{\text{can}} = O(1/n)$. This does *not* mean we observe a value of $O(1/n)$, but means

we observe the definite value 0 with probability $1 - O(1/n)$ which is essentially 1 for large enough n . This is what we mean by (macroscopic) irreversibility [1, 13].

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References

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- [1] We believe that the (still) widespread scenario of obtaining microcanonical distributions from the ergodicity (in the strongest form) can hardly be justified. For careful discussions about these points, see, for examples, J. L. Lebowitz, *Physica A* **194**, 1 (1993); *Physics Today*, Sept. 1993, 32; in *25 Years of Non-Equilibrium Statistical Physics* eds. J. J. Brey et al., *Lecture Notes in Physics* 445, (Springer 1995). Y. Oono, ‘Statistical Thermodynamics’ in *Encyclopedia of Polymer Science and Engineering*, 2nd Edition (John Wiley) vol.15., 614-625 (1989). J. Bricmont, *Physica Magazine* 17, 159-208 (1995), reprinted in *The Flight from Science and Reason* (New York Academy of Sciences, New York, 1996), archived as [chao-dyn/9603009](#).
- [2] We also feel too much emphasis on the possible roles of chaos (either classical or quantum) in the foundation of statistical physics can be misleading. But for attempts to derive statistical distributions using results and conjectures from “quantum chaos”, see M. Srednick, *Phys. Rev. E* **50**, 888 (1994); *J. Phys. A* **29** L75 (1996).
- [3] For numerical experiments which confirm similar scenarios, see R. V. Jensen and R. Shanker, *Phys. Rev. Lett.* **54**, 1879 (1985); K. Saito, S. Takesue and S. Miyashita, *J. Phys. Soc. Jpn.* **65**, 1243 (1996), *Phys. Rev. E* **54**, 2404 (1996). There is a vast literature for situations where an (infinitely large) heat bath is put into an equilibrium distribution (by hand), and time evolution of attached subsystem is discussed.
- [4] Note that (2) is true for *any* operators. Therefore when one “observes” A , one does not see the expectation value itself, but finds fluctuation according to the prediction of the canonical distribution. The origin of the fluctuation may be traced back to the probabilistic interpretation in the Copenhagen spirit. It is correct to say that (at least in the present way of introducing the canonical distribution and within the standard interpretation of quantum mechanics) there is no intrinsic distinction between quantum fluctuation and thermal fluctuation. (Our results themselves are free from any specific interpretations of quantum mechanics.) We stress, however, that the present one is not at all the only reasonable way of introducing probability. See, for examples, [1].

- [5] H. Tasaki, to be published. An unpublished note which (only) contains all the technical details is available as cond-mat/9707255 (or from the author).
- [6] L. D. Landau and E. M. Lifschitz, Quantum Mechanics (Non-relativistic Theory) (Pregamon, 1977).
- [7] Even with the fine structure on H_B , we are not able to control the global solution of (4), and the actual proof is rather involved. In the classically accessible region, we divide the whole range of ℓ into small intervals, and prove in each interval that φ_ℓ has the form suggested by the (discrete version of) quasi-classical analysis [6]; $\varphi_\ell \simeq A \cos(\sum_{\ell'=\ell_0}^{\ell} k_{\ell'} + \theta) / \sqrt{\sin k_\ell}$ with $k_\ell = \cos^{-1}[(E - U_\ell)/\lambda]$. The estimate of the sums in (6) is nontrivial because φ_ℓ oscillates. Near the turning points, we approximate (4) by a continuous equation and estimate φ_ℓ using Bessel's functions. Details can be found in [5].
- [8] The assumption of small energy fluctuation is *physically necessary* no matter how one “derives” the canonical distribution. Without the condition, we end up with a Schrödinger's cat type state where states with different temperatures are superposed.
- [9] Let us restrict ourselves to the non-resonance condition for eigenvalues with $E \geq \varepsilon_n + 2\lambda$ (which is all we need). Suppose that we have a model which violates the non-resonance condition. Then by slightly shifting B_k in the lowest two bands $(0, \delta)$ and $(\delta, 2\delta)$, we get a model which satisfies the condition [5].
- [10] W. Feller, *An Introduction to Probability Theory and Its Applications I*, (Wiley, 1968)
- [11] We took the allowed energy width equal to ε_n only to make formulae simpler. We can prove the corresponding estimates for any energy width. For $c' \simeq 1$ the upper bound for $(\alpha_k)^2$ means that all the allowed basis states in (12) contribute almost equally.
- [12] Macroscopic observables in macroscopic systems automatically have such properties.
- [13] We are *not* trying to get irreversibility from disturbances by observations. We believe it highly misleading to expect any positive roles of observations in (macroscopic) irreversibility and stochastic behavior.